

## PROJECT ADMINISTRATION DATA SHEET

Project No. G 33-616 <sup>misc</sup> ☒ ORIGINAL ☐ REVISION NO. \_\_\_\_\_  
Project Director: E. C. ASHBY School/Dept: Chemistry  
Sponsor: The Petroleum Research Fund, American Chemical Society,  
1155 Sixteenth St N.W., Washington, DC 20036  
Type Agreement: Grant No. 14102-AC4-1C  
Award Period: From 9-1-82 To 8-31-85 (Performance) 8-31-85 (Reports)  
Sponsor Amount: \$ 45,000 Contracted through: \_\_\_\_\_  
Cost Sharing: None GTRI/\_\_\_\_\_ ☒  
Title: Single Electron Transfer in Organic Reactions

## ADMINISTRATIVE DATA

OCA Contact

Don Harty

1) Sponsor Technical Contact:

2) Sponsor Admin/Contractual Matters:

Mr Joseph E. Rogers, Jr  
above address

phone (202) 872-4481

Defense Priority Rating:

N/A

Security Classification:

N/A

## RESTRICTIONS

See Attached

N/A

Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval - Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of \$500 or 125% of approved proposal budget category.

Equipment: Title vests with

N/A - none proposed

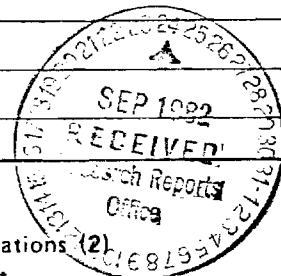
## COMMENTS:

## COPIES TO:

~~Administrative Coordinator~~ RAN  
Research Property Management  
Accounting  
Procurement/EES Supply Services  
FORM OCA 1-77

Research Security Services  
Reports Coordinator (OCA)  
Legal Services (OCA)  
Library

EES Public Relations (2)  
Computer Input  
Project File  
Other \_\_\_\_\_



SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 9/19/86

Project No. G-33-616

School/Lab Chemistry

Includes Subproject No.(s) N/A

Project Director(s) E. C. Ashby

GTRC / ~~GTI~~

Sponsor The Petroleum Research Fund, American Chemical Society

Title Single Electron Transfer in Organic Reactions

Effective Completion Date: 8/31/85 (Performance) \_\_\_\_\_ (Reports) \_\_\_\_\_

Grant/Contract Closeout Actions Remaining:

No further reporting requirements per Ralph Grede.

☒ None

☐ Final Invoice or Final Fiscal Report

☐ Closing Documents

☐ Final Report of Inventions

☐ Govt. Property Inventory & Related Certificate

☐ Classified Material Certificate

☐ Other \_\_\_\_\_

Continues Project No. \_\_\_\_\_

Continued by Project No. \_\_\_\_\_

COPIES TO:

Project Director  
Research Administrative Network  
Research Property Management  
Accounting  
Procurement/GTRI Supply Services  
Research Security Services  
Reports Coordinator (OCAP)  
Legal Services

Library  
GTRC  
Research Communications (2)  
Project File  
Other I. Newton  
A. Jones  
R. Embry



GEORGIA TECH 1885-1985

DESIGNING TOMORROW TODAY

Georgia Institute of Technology  
Grants and Contracts Accounting Dept.  
Lyman Hall/Emerson Building  
Atlanta, Georgia 30332-0259  
Telephone: (404) 894-4624; 2629

May 15, 1986

Joseph E. Rodgers, Jr.  
The Petroleum Research Fund  
American Chemical Society  
1155 Sixteenth Street, N.W.  
Washington, D. C. 20036

Gentlemen:

Enclosed in duplicate is the Annual Financial Statement and Personnel Statement for PRF No. 14102-AC4-1C for the year ended August 31, 1985.

If you have questions or require any additional information, please contact this office at (404) 894-5523.

Sincerely,

Valeria D. Henderson, Accountant I  
Grants & Contracts Accounting

VDH/djt

Enclosures

cc: Dr. R. A. Pierotti/Chemistry  
Dr. E. C. Ashby/Chemistry  
~~Ms. Faith Gleason/OCA-PAD~~  
File G-33-616 (R5532-1A0)

FINANCIAL STATEMENT  
(Insert "ANNUAL" or "FINAL", as appropriate)

AMERICAN CHEMICAL SOCIETY - THE PETROLEUM RESEARCH FUND

For the Period: September 1, 1984 to August 31, 1985  
(The preferred closing date for the reporting period is August 31.)

Balance Carried Over from Previous Reporting Period (from Same or Earlier Grant)	\$ 14,007.50
Received from PRF During Report Period (Include Supplements)	- 0 -
Stipends to:	
a. Principal Investigator . . . . . (Contribution Toward Summer Salary*)	
b. Undergraduate Students . . . . .	
c. Graduate Students . . . . .	14,604.88
d. Postdoctoral Fellows . . . . .	
e. Summer Research Fellows (Only if funded by Summer Research Supplement) Faculty <input type="checkbox"/> Student <input type="checkbox"/> (check one) . .	
f. Other (Specify) Research Sci. . . . .	
Tuition . . . . .	
Materials and Supplies . . . . .	(1,097.38)
Equipment . . . . .	
Computer Time Charges . . . . .	
Travel (Explain if in excess of budget) . . . .	
Other Expenses (Attach itemized list) . . . . .	
Departmental Allocation* . . . . .	500.00
*If provided in grant agreement	
Total Expenditures During Reporting Period . .	14,007.50
Balance on Hand at End of Period	- 0 -
Total of PRF Grant Payments Received to Date	45,000.00

Complete this section only for a FINANCIAL STATEMENT which shows a balance in the grant account at the termination date of the current grant agreement.

The balance in the grant account will be liquidated:

☐ By refund of unspent and uncommitted funds. The check should be drawn to the order of American Chemical Society - The Petroleum Research Fund, and identified by the number of the grant.

☐ By use in the completion of the grant project. We hereby request approval by the American Chemical Society of an extension of the grant agreement, without commitment of additional funds, until \_\_\_\_\_ (Period up to one year, renewable).

We certify that the expenses reported herein were incurred for education and research in accord with the terms of the approved ACS-PRF grant-in-aid.

Georgia Institute of Technology  
(Grantee Institution)

<u>Valeria D. Henderson</u>	<u>(404) 894-5523</u>	<u>5/15/86</u>
Financial Officer (typed name)	(Signature)	(Telephone)
		(Date)

<u>E. C. Ashby</u>	<u>14102-AC4-C</u>
Name of Principal Investigator	PRF Number

Please submit to The Petroleum Research Fund, American Chemical Society  
1155 Sixteenth Street, N.W., Washington, D.C. 20036 Telephone (202) 872-4481

PERSONNEL STATEMENT

PRF# 14102-AC4-1C REPORTING PERIOD September 1, 1984 TO August 31, 1985  
GRANTEE INSTITUTION Georgia Institute of Technology DEPARTMENT Chemistry  
PRINCIPAL INVESTIGATOR (S) E. C. Ashby  
GRANT PROJECT TITLE Single Electron Transfer in Organic Reactions

List undergraduate, graduate, and postdoctoral co-workers receiving stipends under the above named grant:

NAME	TITLE OR ACADEMIC APPOINTMENT	PREVIOUS EDUCATION & DEGREES*	COUNTRY OF PERMANENT RESIDENCE	PERIOD OF SUPPORT (MONTHS)	PERCENT OF SUPPORT FROM PRF	DEGREES RECEIVED (IF ANY) DURING REPORTING PERIOD
Argyropoulos, John	Graduate Research Asst	Yale, MS	USA	1.5	100% (1.5 mo)	PHD Ga Tech, 1986
Baldwin, R. Keith	Graduate Teaching Asst	UGA, BS	USA	1	100% 1 mo)	None
Coleman, David	Graduate Teaching Asst	GA Tech, BS	USA	4	100% (4 mo)	PHD GA Tech, 1986
Park, Bong-Jin	Graduate Research Asst	Portland	Korea	8	50% (3 mos) 100% (5 mos)	None

List other co-workers on grant project not directly supported with ACS - PRF funds:

NAME	SOURCE OF SUPPORT	DATES ASSOCIATED WITH GRANT PROJECT

For graduate students, indicate the College or University attended prior to graduate work. For postdoctoral fellows, give the name of the Ph. D. granting institution.

PERSONNEL STATEMENT

PRF# 14102-AC4-1C REPORTING PERIOD September 1, 1984 TO August 31, 1985  
 GRANTEE INSTITUTION Georgia Institute of Technology DEPARTMENT Chemistry  
 PRINCIPAL INVESTIGATOR (S) E. C. Ashby  
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Oswald, John	Graduate Teaching Asst	BS Chem Ga Tech	USA	1	100% ( 1 mo)	None
Pham, Tung-Ngoc	Graduate Research Asst	BS Chem U. of Saigon	USA	7	100% ( 7 mos)	None

List other co-workers on grant project not directly supported with ACS - PRF funds:

NAME	SOURCE OF SUPPORT	DATES ASSOCIATED WITH GRANT PROJECT

For graduate students, indicate the College or University attended prior to graduate work. For postdoctoral fellows, give the name of the Ph. D. granting institution.

REPORT ON ACTIVITY ASSISTED BY

GRANT, PRF # 14102-AC4-C

Page 1 of 1 pages.

PREPARED BY

E. C. Ashby

Date June 16, 1986

Please refer to instructions.

Fill in information requested  
above for each page.

The report heading, narrative,  
and all drawings must be prepared  
within the box.

Please submit one sharp, clear  
"original" and a copy (Xerox,  
carbon, etc.) for each page.

Single Electron Transfer in Organic  
Reactions

E. C. Ashby, Georgia Institute of  
Technology, Atlanta, Georgia 30332

Halogen-metal exchange has been studied by allowing t-Butyllithium to react with a series of alkyl halides containing a cyclizable radical probe in order to evaluate the occurrence of a radical intermediate in the reaction. It was found that radical intermediates, formed via a single electron transfer pathway, are involved in the reactions of t-BuLi with the radical probe, (endo)-5-(2'-bromoethyl)-2-norbornene in pentane: Et<sub>2</sub>O at -78°C, since cyclized hydrocarbons were formed during the reaction. However, there was no evidence to support an electron transfer pathway in reactions of the corresponding iodide and chloride with t-BuLi under the same conditions since only the straight-chain organolithium compound was formed. However evidence indicative of a radical intermediate was obtained from reactions of the iodo compound with t-BuLi in pentane:Et<sub>2</sub>O at higher temperatures (-45° and -23°) and in pure pentane at -78°C and -23°C in which stable cyclized hydrocarbon product was obtained. Lithium complexing agents such as TMEDA, HMPA and 18-crown-6 were employed in these reactions in order to increase the carbanionic nature of the organolithium products. It was found that cyclization of the straight-chain organolithium compound to the corresponding cyclized organolithium compound in the presence of such complexing agents is relatively slow. On the other hand, the effectiveness of the complexing agents to increase carbanion character of the straight-chain organolithium compound was demonstrated by a significant lowering of the deuterium content of the straight-chain product due to ether cleavage by the straight-chain organolithium compound.